

**REMARKS**

By this amendment, claim 1 is amended. These amendments are made to even more clearly recite the claimed invention, do not add prohibited new matter and are fully supported by the specification. For example, support for the amendment of the preamble of claim 1 can be found on page 11, lines 9-19; support for the remaining amendments can be found for example, on page 7, lines 23-29, on page 12, line 31 through page 13, line 5, in Figure 4, and on page 6, lines 13-19. Reconsideration and withdrawal of the rejections in the outstanding Office Action are respectfully requested in view of the foregoing amendments and the following remarks.

**Claim Rejections – 35 U.S.C. § 101**

Claims 1, 6, and 11 are rejected under 35 U.S.C. § 101 for allegedly being directed to non-statutory subject matter.

With the present amendment, Applicants respectfully request withdrawal of this rejection. Applicants respectfully submit that the present amendment claims a method that “is [tied] to a particular machine or apparatus,” which in view of *Bilski v. Warsaw* constitute patent-eligible subject matter.

**Claim Rejections – 35 U.S.C. § 102**

The Office Action rejects claims 1, 6, 7, and 11 under 35 U.S.C. 102(b) as being anticipated by Wang et al. (J. Med. Chem., Vol. 37, pp. 4479-4489 (1994), hereinafter “WANG”).

In view of the present amendment, Applicants respectfully submit that WANG does not anticipate the claimed invention. Applicants note that step c.) of claim 1 has been amended to even more clearly recite the binding scheme of lead-candidate compounds to the protein based on the three-dimensional structures of the lead-candidate compounds and the protein.

Applicants note that WANG does not disclose at least this feature. In particular, Applicants respectfully submit that WANG does not disclose “estimating a binding scheme,” which is “based on the three-dimensional information of the query molecule, the binding scheme of the query molecule

to the protein.” In the absence of the recited feature of claim 1, there can be no anticipation. Applicants respectfully request withdrawal of the § 102 rejection.

**CONCLUSION**


In view of the foregoing, Applicant submits that the Examiner’s rejections should be withdrawn. Entry and consideration of the present amendment, reconsideration of the outstanding Office Action, and allowance of the present application and all of the claims therein are respectfully requested and now believed to be appropriate.

Any amendments to the claims which have been made in this amendment, and which have not been specifically noted to overcome a rejection based upon the prior art, should be considered to have been made for a purpose unrelated to patentability, and no estoppel should be deemed to attach thereto.

Should the Commissioner determine that any extension of time is required in order to render this response timely and/or complete, including any extension required for entry of an Examiner’s amendment, the Commissioner is authorized to charge such required extension of time fee under 37 C.F.R. §1.17 to Deposit Account No. 19-0089.

If the Examiner has any questions, or wishes to discuss this matter, the Examiner is respectfully requested to contact the undersigned at the below-listed telephone number.

Respectfully submitted,  
A. ITAI et al.

  
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